S_N2 Mechanism

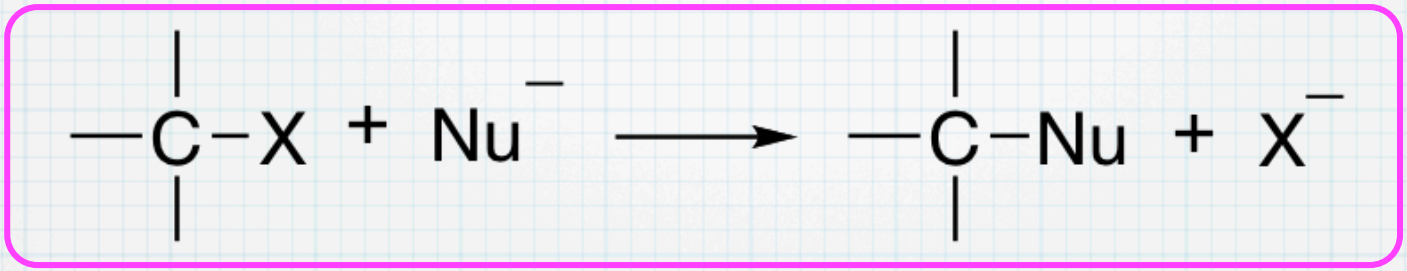
UCI Chem 51A
Dr. Link

Goals

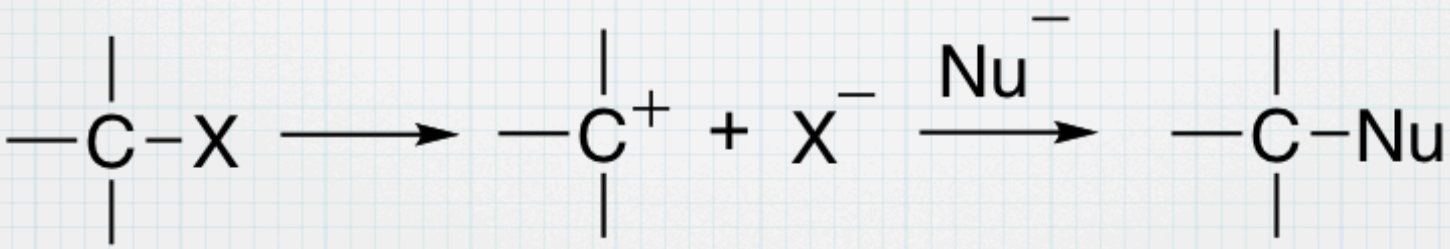
- After this lesson you should be able to:
  - Identify and draw an S_N2 reaction mechanism
  - Describe the experimental evidence that supports the S_N2 mechanism
  - Identify electrophiles that are likely to undergo SN2 reactions
  - Explain the importance of the leaving group in an SN2 reaction
  - Identify nucleophiles that favor SN2 reactions
  - Explain the effect of solvent on SN2 reactions
  - Describe the consequences of an SN2 reaction occurring at a carbon that is also a stereocenter.

Two Mechanisms for Substitution

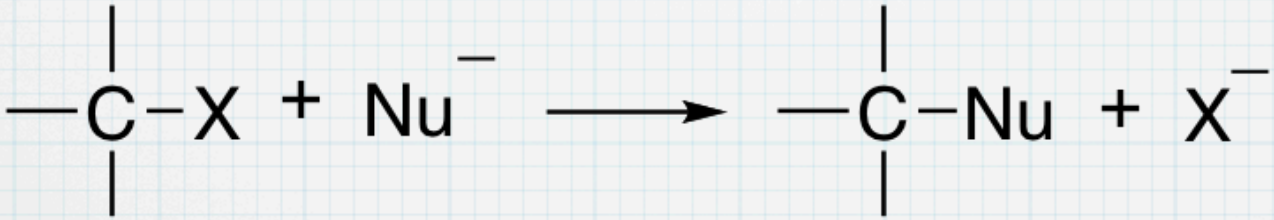
All at once:

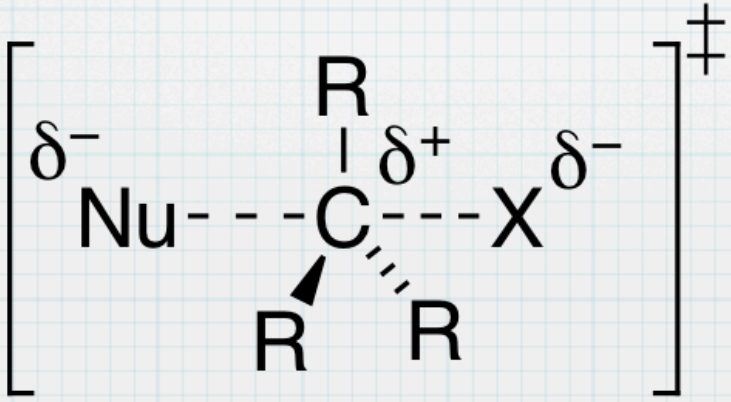


Break, then form:



The S_N2 Mechanism





How Do We Know?

Rates rate = k [E] [Nu]

Rate law derived experimentally.

Nucleophile & electrophile both involved in RDS.

Intermediates

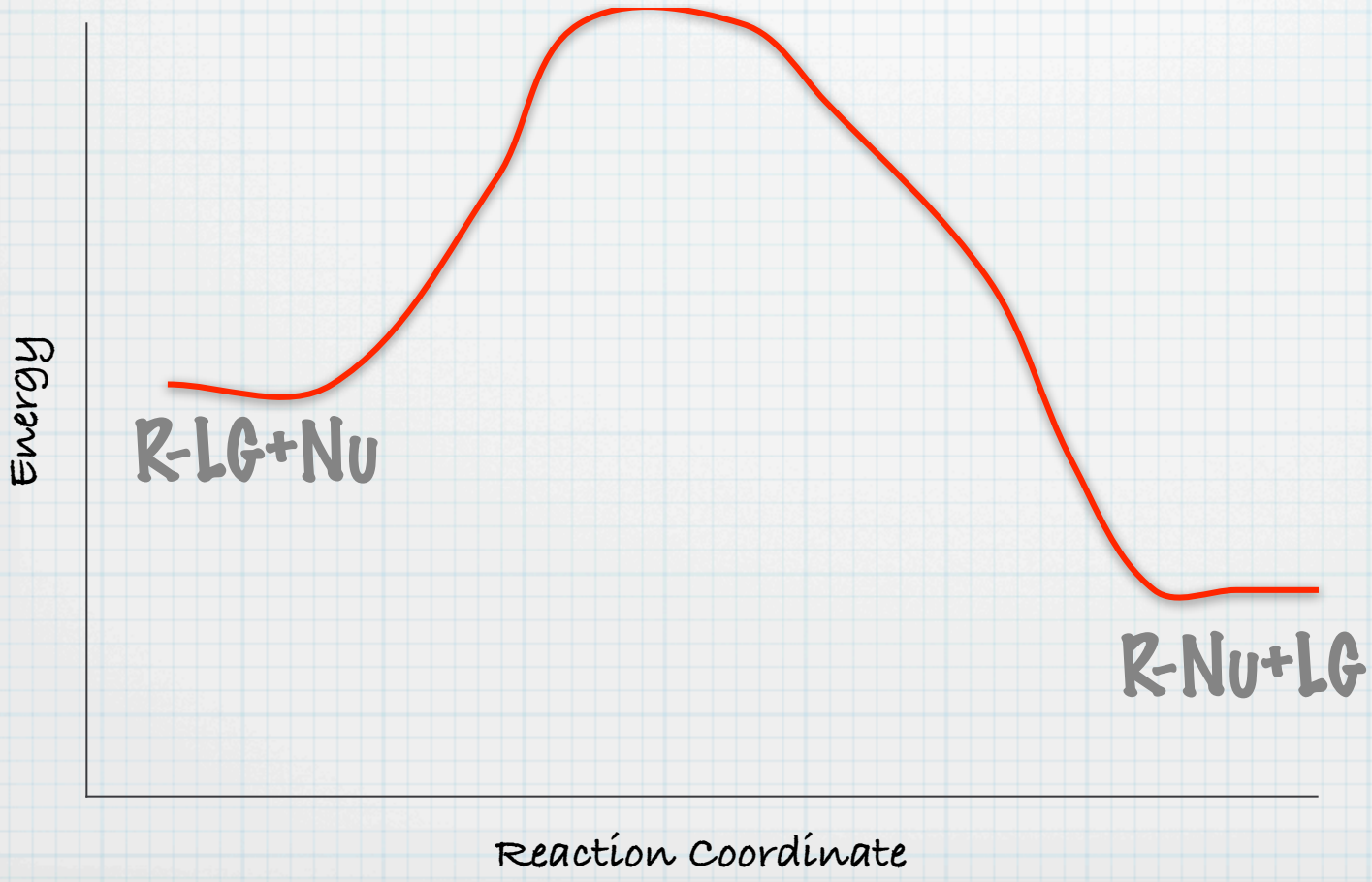
No intermediates identified experimentally.

Stereochemistry

Effects on stereocenters support S_N2

The Leaving Group

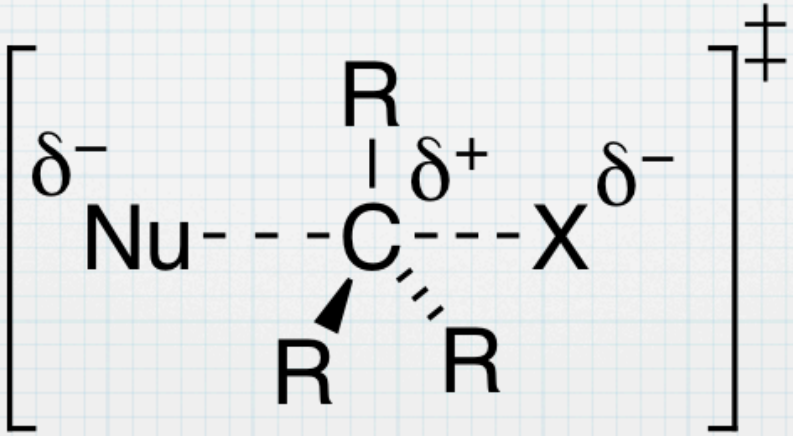
* All nucleophilic substitution reactions require a good leaving group.



The Electrophilic Carbon

Type of C matters

Why? Sterics!



The Nucleophile

* S_N2 reactions are favored by STRONG nucleophiles

S_N2 reactions in competition

Strong Nu means faster rate for S_N2
More likely to out-compete other rxns

Common S_N2 Nu

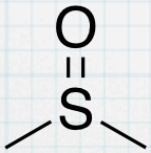
RO^- CN^- RS^- X^-

The Solvent

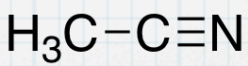
* S_N2 reactions are favored by POLAR APROTIC solvents

acetone

tetrahydrofuran (THF)



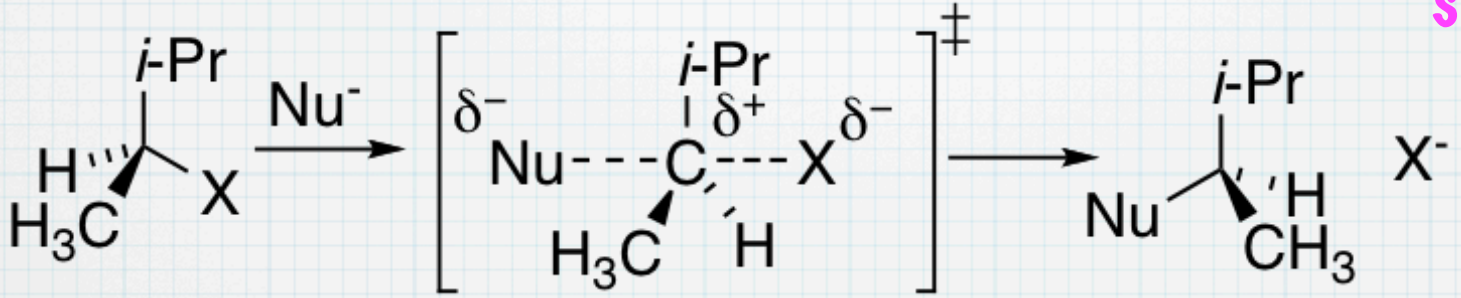
dimethyl sulfoxide (DMSO)



acetonitrile

Stereochemistry and S_N2 Mechanism

* Inversion!



stereocenter inverted!

Why?

S_N2 Summary

* Rate = 2nd order
* Mechanism = 1 step
* Electrophile: Me>1°>2°, no 3°
* LG = good LG required
* Nu = strong Nu favors S_N2
* Solvent: polar aprotic favors S_N2
* Stereochemistry: backside attack, inversion

Nice summary video!

http://www.youtube.com/watch?NR=1&feature=endscreen&v=h5xvaP6blZI

Wrapping Up

- Practice drawing mechanisms for S_N2 reactions
- Practice predicting which electrophiles are most likely to undergo S_N2 reactions
- Practice identifying electrophiles with good leaving groups
- Practice drawing the products for an S_N2 reaction at a stereocenter